Supplementary Table

Supplementary Table 2 The ADME data of compounds

Compound	Molecular formula	Freely Rotating Bonds	H bond acceptors	H bond donors	logP	Molecular Weight
2α,3α,23-trihydroxyurs-12-en-28-oic acid	$C_{30}H_{48}O_5$	5	5	4	5.748±0.425	488.7
3β,23-dihydroxy-12-ene-28-ursolic acid	$C_{30}H_{46}O_3$	1	3	1	7.633±0.573	454.68
2α-hydroxyursolic acid	$C_{30}H_{48}O_4$	3	4	3	7.113±0.412	472.7
2α,3α,23-trihydroxyurs-12,20(30)-dien-28-oic acid	$C_{30}H_{46}O_5$	5	5	4	4.787±0.436	486.68
2α,3β,23-trihydroxy-12-ene-28-ursolic acid	$C_{30}H_{48}O_5$	5	5	4	5.748±0.425	488.7
3β-O-trans-caffeoyl-morolic acid	$C_{39}H_{54}O_6$	7	6	3	11.175±0.463	618.84
actinidic acid	$C_{30}H_{46}O_5$	5	5	4	4.787±0.436	486.68
arjunolic acid	$C_{30}H_{48}O_5$	5	5	4	5.593±0.442	488.7
corosolic acid	$C_{30}H_{48}O_4$	3	4	3	7.113±0.412	472.7
Cyclocaric acid B	$C_{30}H_{46}O_5$	4	5	3	5.010±0.495	486.68
daucosterol	$C_{35}H_{60}O_6$	13	6	4	8.615±0.345	576.85
Hederagenin	$C_{30}H_{48}O_4$	4	4	3	7.065±0.404	472.7
maslinic acid	$C_{30}H_{48}O_4$	3	4	3	6.958±0.430	472.7
olean-12-en-28-oic acid	$C_{30}H_{48}O_3$	1	2	1	10.457±0.388	440.7
oleanolic acid	$C_{30}H_{48}O_3$	2	3	2	8.576±0.394	456.7
taraxerol	$C_{30}H_{50}O$	1	1	1	10.481±0.383	426.72
β-amyrin	$C_{30}H_{50}O$	1	1	1	10.481±0.383	426.72
β-amyrone	$C_{30}H_{48}O$	0	1	0	10.019±	424.7

β-sitosterol	$C_{29}H_{50}O$	7	1	1	0.433 10.482±0.287	414.71
cyclocariosides I	$C_{35}H_{56}O_8$	14	8	5	6.018±0.629	604.81
cyclocarioside N	$C_{44}H_{74}O_{13}$	14	13	6	5.294±0.807	811.05
3β, 23-dihydroxy-1,12-dioxo-olean-28-oic acid	$C_{30}H_{46}O_6$	4	6	3	2.287±0.507	502.68
3β,23,27-trihydroxy-1-oxo-olean-12-ene-28-oic acid	$C_{30}H_{46}O_6$	6	6	4	1.993±0.475	502.68
2α,3β,23-trihydroxyurs-11-oxo-12-ene-28-oic acid	$C_{30}H_{46}O_6$	5	6	4	3.484±0.439	502.68
Cyclocarioside II	$C_{35}H_{36}O_8$	15	8	5	6.158±0.642	604.81
arjunglucoside II	$C_{36}H_{58}O_{10}$	12	10	7	4.165±0.631	650.84
quadranoside IV	$C_{36}H_{58}O_{10}$	12	10	7	4.320±0.619	650.84
α-boswellic acid	$C_{30}H_{48}O_3$	2	3	2	8.949±0.406	456.7
3α,4β,18α-3-Hydroxyurs-12-en-23-oic acid	$C_{30}H_{48}O_3$	2	3	2	9.105±0.387	456.7
β-boswellic acid	$C_{30}H_{48}O_3$	2	3	2	9.105±0.387	456.7
Cyclocarioside H	$C_{43}H_{72}O_{13}$	15	13	6	4.929±0.845	797.02
cyclocarioside J	$C_{35}H_{58}O_9$	16	9	6	4.624±0.633	622.83
2α,3β,23- trihydroxyoleana-11,13(18)-dien-28-oic acid	$C_{30}H_{46}O_5$	5	5	4	4.618±0.507	486.68
Cyclocaric acid A	$C_{30}H_{46}O_3$	1	3	1	8.257±0.416	454.68
(+)-Betulinic acid	$C_{30}H_{48}O_3$	3	3	2	7.653±0.421	456.7
cyclocarioside K	$C_{41}H_{70}O_{12}$	13	12	7	3.914±0.804	754.99
Cyclocarioside III	$C_{36}H_{60}O_9$	12	9	5	5.062±0.650	636.86
cyclocarioside L	$C_{38}H_{62}O_{12}$	12	12	6	3.867±0.707	710.89
cyclocarioside M	$C_{40}H_{64}O_{13}$	13	13	5	4.287±0.848	752.93

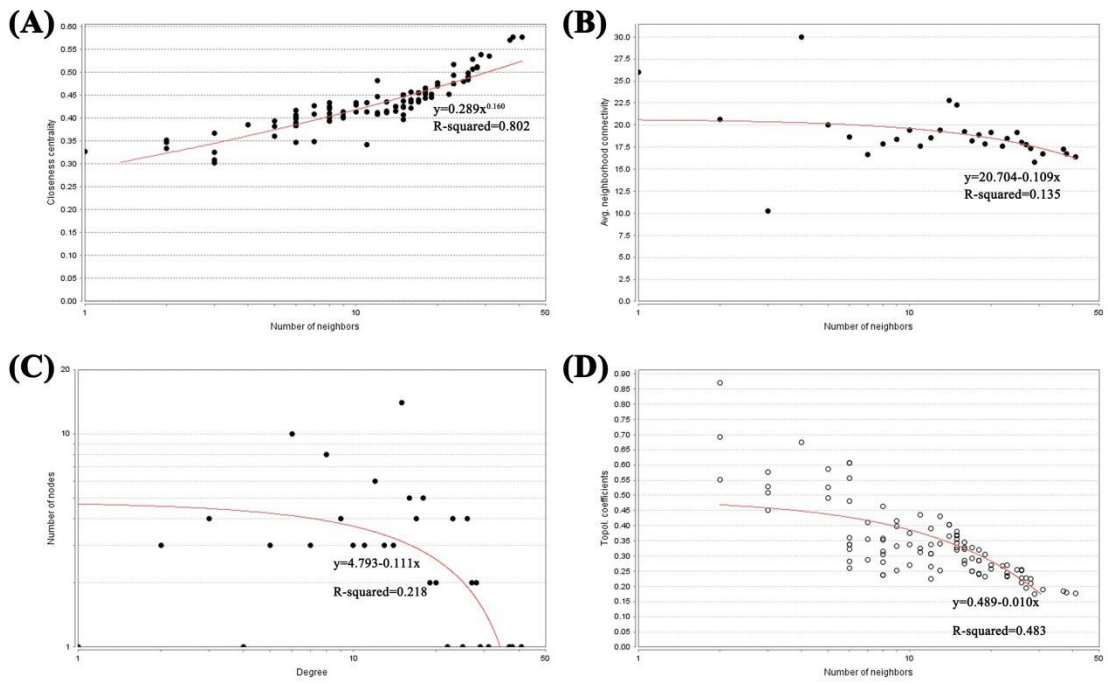
Supplementary Table 3 The result data of component-target-pathway network

Name	Betweenness Centrality	Closeness Centrality	Degree layout	Neighborhood Connectivity	Topological Coefficient
M39	0.00	0.33	2.00	18.00	0.69
M38	0.01	0.46	18.00	20.17	0.28
M37	0.01	0.46	18.00	20.17	0.28
M36	0.03	0.51	27.00	18.19	0.23
M35	0.01	0.38	6.00	23.17	0.56
M34	0.03	0.48	20.00	20.10	0.27
M33	0.01	0.41	9.00	17.89	0.33
M32	0.00	0.41	12.00	17.17	0.31
M31	0.00	0.41	12.00	17.17	0.31
M30	0.02	0.45	17.00	16.88	0.25
M29	0.02	0.45	17.00	16.88	0.25
M28	0.03	0.46	18.00	16.11	0.24
M27	0.04	0.51	28.00	16.71	0.21
M26	0.04	0.51	28.00	18.00	0.22
M25	0.01	0.45	19.00	20.68	0.30
M24	0.03	0.46	16.00	21.56	0.33
M23	0.02	0.39	8.00	11.13	0.24
M22	0.02	0.39	8.00	11.13	0.24
M21	0.02	0.44	19.00	15.05	0.23
M20	0.08	0.58	38.00	16.74	0.18
M19	0.01	0.41	9.00	13.67	0.25
M18	0.01	0.41	7.00	22.00	0.41
M17	0.01	0.43	10.00	20.10	0.34
M16	0.01	0.43	11.00	19.45	0.31
M15	0.01	0.45	15.00	24.00	0.37
M14	0.01	0.45	15.00	24.00	0.37
M13	0.01	0.45	15.00	24.00	0.37
M12	0.01	0.45	15.00	24.00	0.37
M11	0.03	0.49	26.00	18.73	0.25
M10	0.01	0.45	15.00	24.00	0.37
M9	0.00	0.41	8.00	24.75	0.46
M8	0.00	0.38	6.00	25.17	0.61
M7	0.00	0.38	6.00	25.17	0.61
M6	0.05	0.48	26.00	16.96	0.23
M5	0.01	0.45	15.00	24.00	0.37
M4	0.01	0.45	15.00	24.00	0.37

M3	0.00	0.39	5.00	20.60	0.49
M2	0.01	0.45	15.00	24.00	0.37
M1	0.01	0.45	15.00	24.00	0.37
VEGFA	0.00	0.45	12.00	18.50	0.26
VDR	0.01	0.43	10.00	17.20	0.27
STAT3	0.01	0.52	23.00	22.00	0.24
SHBG	0.00	0.35	6.00	10.00	0.36
SCD	0.00	0.37	3.00	14.00	0.45
PTPRF	0.00	0.42	16.00	14.63	0.29
PTPN1	0.04	0.54	29.00	15.79	0.18
PTGS2	0.00	0.43	8.00	17.38	0.28
PPARG	0.00	0.43	7.00	18.14	0.29
PPARD	0.00	0.42	6.00	20.00	0.34
PPARA	0.00	0.42	8.00	17.75	0.31
PIK3CA	0.03	0.53	27.00	17.44	0.19
NR3C1	0.00	0.33	3.00	10.67	0.51
NR1H4	0.00	0.30	3.00	7.33	0.58
NOS2	0.01	0.47	20.00	18.25	0.26
MAPK14	0.01	0.44	18.00	15.83	0.24
KDR	0.00	0.40	6.00	16.83	0.32
IL2	0.00	0.43	8.00	24.38	0.36
IKBKB	0.02	0.48	23.00	17.35	0.23
HSD11B2	0.00	0.35	2.00	28.00	0.87
HSD11B1	0.04	0.49	23.00	14.57	0.23
HMGCR	0.00	0.40	6.00	15.00	0.28
FGF2	0.00	0.40	8.00	17.63	0.31
FABP4	0.00	0.36	5.00	14.20	0.53
FABP2	0.00	0.31	3.00	9.00	0.53
F2	0.00	0.39	4.00	30.00	0.67
ESR1	0.00	0.38	6.00	14.50	0.34
CYP19A1	0.00	0.35	7.00	9.86	0.35
CNR1	0.00	0.35	2.00	16.00	0.55
CASP3	0.01	0.48	12.00	19.00	0.22
AR	0.00	0.41	6.00	14.33	0.26
AKR1B1	0.00	0.33	1.00	26.00	0.00
ACP1	0.01	0.41	15.00	14.13	0.33
hsa05133	0.01	0.44	16.00	17.38	0.28
hsa05152	0.06	0.50	26.00	16.69	0.21
hsa05140	0.01	0.40	15.00	15.73	0.32
hsa04920	0.01	0.44	15.00	22.27	0.34

hsa05206	0.01	0.44	17.00	20.59	0.33
hsa05120	0.00	0.39	6.00	22.67	0.48
hsa04210	0.00	0.38	5.00	25.20	0.59
hsa04932	0.00	0.40	9.00	20.67	0.40
hsa05161	0.00	0.42	13.00	24.08	0.43
hsa04923	0.01	0.40	8.00	18.75	0.35
hsa04550	0.01	0.43	15.00	21.40	0.36
hsa04910	0.05	0.54	31.00	16.71	0.19
hsa04068	0.00	0.43	14.00	24.14	0.40
hsa04380	0.01	0.41	10.00	21.00	0.38
hsa04152	0.02	0.44	13.00	16.15	0.25
hsa04014	0.00	0.41	12.00	20.42	0.39
hsa04151	0.01	0.42	14.00	20.07	0.36
hsa05169	0.00	0.43	14.00	24.14	0.40
hsa04660	0.00	0.41	11.00	24.36	0.44
hsa04066	0.02	0.48	25.00	19.16	0.26
hsa05222	0.01	0.44	17.00	18.41	0.29
hsa04917	0.01	0.44	16.00	20.31	0.32
hsa05212	0.00	0.42	15.00	22.47	0.38
hsa05160	0.01	0.45	18.00	22.11	0.32
hsa04015	0.01	0.41	13.00	18.08	0.34
hsa05221	0.01	0.44	16.00	22.44	0.35
hsa05145	0.02	0.49	26.00	19.77	0.25
hsa04668	0.00	0.40	9.00	21.22	0.42
hsa05142	0.02	0.48	23.00	19.96	0.27
hsa04370	0.01	0.41	12.00	18.92	0.34
hsa04931	0.08	0.57	37.00	17.30	0.18
hsa05205	0.02	0.45	22.00	17.59	0.27
hsa03320	0.01	0.34	11.00	9.09	0.32
hsa05200	0.12	0.58	41.00	16.39	0.18

Supplementary Figure



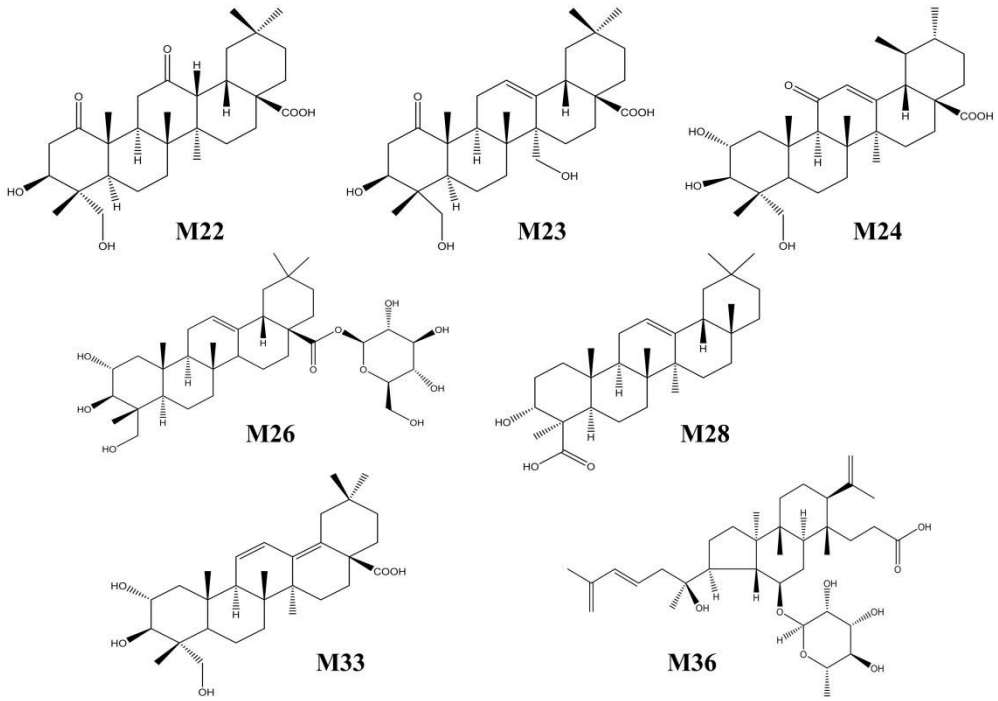
Supplementary Figure 1 The figures of network analysis graph

（A）Closeness centralities

（B）Neighborhood connectivity distribution

（C）Node degree distribution

（D）Topological coefficient



Supplementary Figure 2 The structure of the seven potential active compounds from *Cyclocarya paliurus*. M22: 3β, 23-dihydroxy-1,12- dioxo-olean-28-oic acid; M23: 3β,23,27- trihydroxy-1-oxo-olean-12-ene-28-oic acid; M24: 2α,3β,23-trihydroxyurs-11-oxo-12-ene- 28-oic acid; M26: arjunglucoside II; M28: α-boswellic acid; M33:2α,3β,23-trihydroxyoleana-11,13(18)-dien-28-oic acid; M36: cyclocarioside K.